

The Location of the CO₂ Fundamental in Clathrate Hydrates and its Application to Infrared Spectra of Icy Solar System Objects

S. A. Sandford, R. M. E. Mastrapa, M. P. Bernstein, D. P. Cruikshank
NASA Ames Research Center

CO₂ is present on the surface of many Solar System objects, but not always as a segregated, pure ice. In pure CO₂-ice, the fundamental absorption is located near 4.268 μm (2343.3 wavenumbers). However, on several objects, the CO₂ fundamental is shifted to higher frequency, (Table 1). This shift may be produced by CO₂ gas trapped in another material, or adsorbed onto minerals. We have seen that a mixture of H₂O, CH₃OH, and CO₂ forms a type II clathrate when heated to 125 K and produces a CO₂ fundamental near 4.26 μm (Blake, et al. 1991). The exact location of the feature is strongly dependent on the initial ratio of the three components, (Table 1).

We are currently exploring various starting ratios relevant to the Solar System to determine the minimum amount of CH₃OH needed to convert all of the CO₂ to the clathrate, i.e. eliminate the splitting of the CO₂ fundamental. We are testing the stability of the clathrate to thermal processing and UV photolysis, and documenting the changes seen in the spectra in the wavelength range from 1-5 μm . We acknowledge financial support from the Origins of Solar Systems Program, the Planetary Geology and Geophysics and the NASA Postdoctoral Program.

Table 1. Location of CO₂ Fundamental in the Solar System and the Laboratory

Object	Lab Sample	Shift of CO ₂ From 2343.3 cm ⁻¹
	H ₂ O:CO ₂	-4.3,+15.7*
Ganymede		+5.8
Callisto		+5.2
Phoebe		+3.7
Iapetus		+3.7
	H ₂ O:CH ₃ OH:CO ₂ (100:2.5:1)	+3.3, -3.3*
	H ₂ O:CH ₃ OH:CO ₂ (100:10:5)	+3.5, -6.1*
	H ₂ O:CH ₃ OH:CO ₂ (100:50:1)	+2.7

* Splitting of fundamental absorption.

Blake, D. F., L. Allamandola, et al. (1991). "Clathrate hydrate formation in amorphous cometary ice analogs in vacuo." *Science* **254**: 548-551.